Analysis of a diffuse-domain approach to handle complex geometries

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Technische Universität Dresden

Prague, 13/04/2012

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A note on the Analysis of a diffuse-domain approach to handle complex geometries

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Overview

Introduction

Consider an elliptic differential equation of second order given by

$$Lu = f \quad \text{in } \Omega, \qquad u = g \quad \text{on } \partial\Omega.$$

for a given geometry $\Omega \subset \mathbb{R}^n$, $n = 1, 2, 3$.
Here Ω might be some *complicated subset or manifold* embedded in $\mathbb{R}^n$. A straightforward numerical approach to solve this problem numerically requires an *appropriately chosen mesh* of the domain Ω. For complicated domains the task of finding a suitable mesh becomes challenging and is one of the most time consuming parts in computational engineering.

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An alternative is to embed the problem into a larger, but simpler domain $\widehat{\Omega}$ and modify the differential equation.

The approach we want to use is called *diffuse-domain approximation*. It describes the domain Ω *implicitly*, using a phase-field function Φ, given by

$$\Phi(x) = \frac{1}{2}\left(1 - \tanh\left(\frac{r(x)}{\mu}\right)\right).$$

Here $0 < \mu \ll 1$ is a small parameter and $r(x)$ the signed-distance function measuring the distance between x and $\partial\Omega$.

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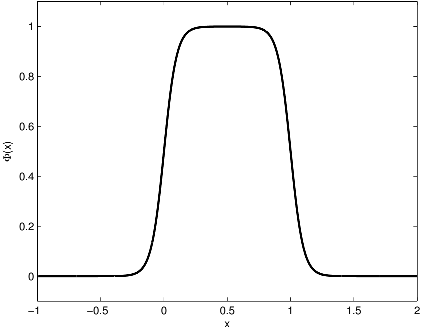

Phase-field function Φ for the signed-distance function $r(x) = \max\{-x, x-1\}$ and $\mu = 0.1$.

Introduction

Let us assume the simple problem $Lu = -\Delta u + cu = f$ in Ω with $c \geq \gamma \geq 0$ and $u = g$ on $\partial\Omega$. Moreover, assume all data to be smooth.

Then the diffuse domain approximation is given by

$$L_\mu u_\mu = -\nabla \cdot (\Phi \nabla u_\mu) + \Phi c u_\mu + \frac{1-\Phi}{\mu^\alpha} u_\mu = \Phi f + \frac{1-\Phi}{\mu^\alpha} g \quad \text{in } \widehat{\Omega},$$
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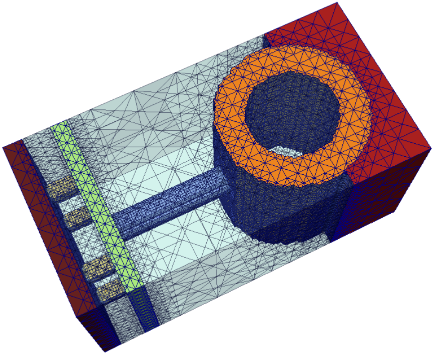
Examples – Ion Channel in Cell Surface

Work done by group of A. Voigt, IWR TU Dresden



7 phase fields used to describe diffuse domain

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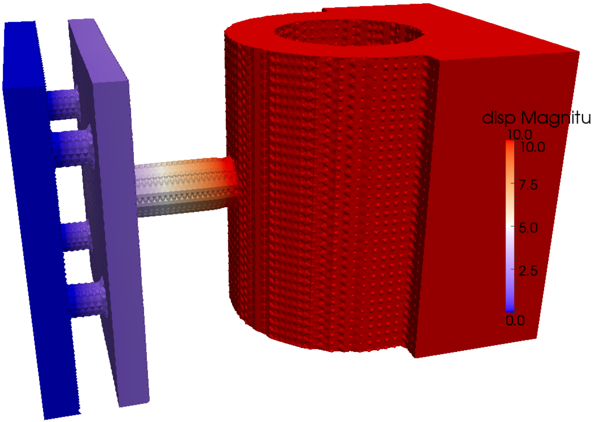

Computed displacement

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Examples – Structure of Bones

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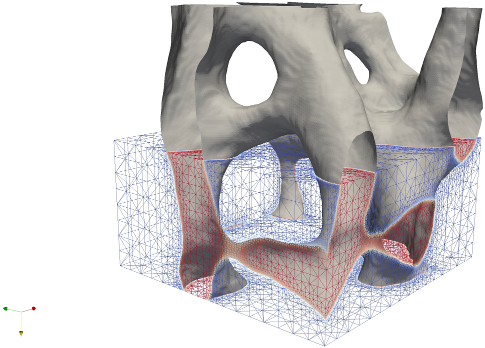

Phase field function generated from tomography data

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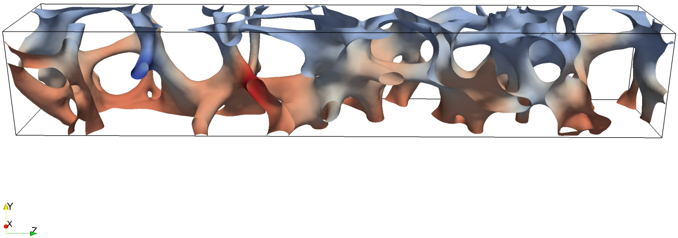

Solution component of elasticity equations

Examples – Navier-Stokes Equations

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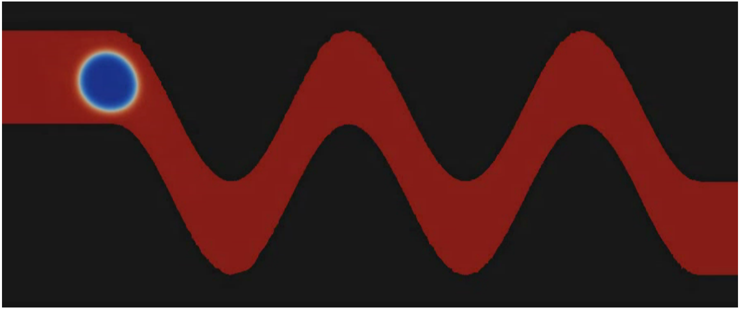

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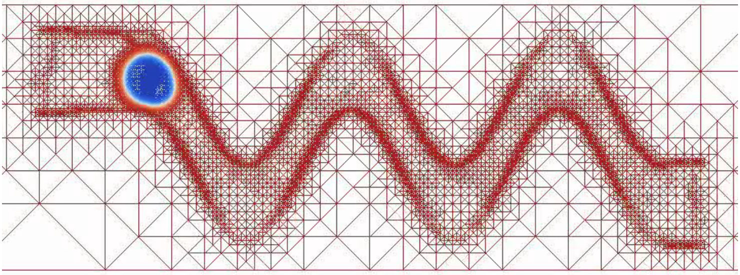

Examples – Sliding Raindrop

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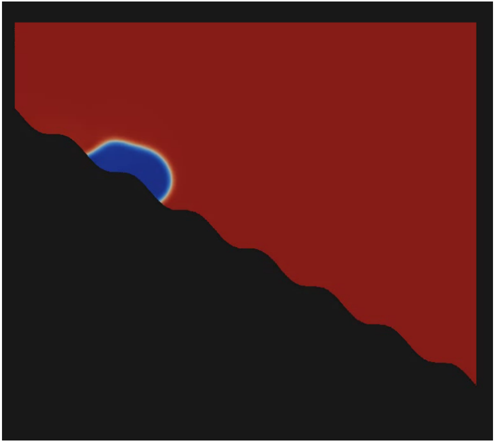

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We consider the following *one-dimensional* model problem

$$Lu := -u'' + cu = f \quad \text{in } \Omega = (0,1)$$
$$u(0) = A,\ u(1) = 0,$$

and apply the diffuse-domain approach *only to the left boundary condition*. We set $\widehat{\Omega} = (-1,1)$.
Then the appropriate phase-field function Φ is given by

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Thus, our diffuse-domain approach reads

$$L_\mu u_\mu := -(\Phi u_\mu')' + \Phi c u_\mu + \frac{1-\Phi}{\mu^\alpha} u_\mu = \Phi f + \frac{1-\Phi}{\mu^\alpha} A \quad \text{in } \widehat{\Omega}$$

$$u_\mu(-1) = A, \quad u_\mu(1) = 0.$$

Analysis – Step 1

Lemma (Existence and Uniqueness)

For each $\mu > 0$ and $\alpha > 0$ exists a unique solution u_μ.

Proof.

Classical existence theory. □

Lemma (Boundedness)

The solution u_μ is bounded uniformly with respect to μ and α.

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Barrier function and maximum principle. □

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Lemma

For $\alpha > 2$, $\theta > 0$ arbitrary but fixed and $\mu < \mu_0$, where μ_0 is sufficiently small, we have

$$u_\mu(x) = A + \mathcal{O}\left(\mu^\alpha\right) \quad \textit{for } x \in [0, \theta\mu].$$

Proof. By scaling $\xi = x/\mu$ we obtain in $(-1, \theta + 1)$ the scaled problem

$$-\mu^{\alpha-2}\frac{\partial}{\partial\xi}\left(\tilde{\Phi}\frac{\partial}{\partial\xi}\tilde{u}_\mu\right) + \left[\mu^\alpha\tilde{\Phi}\tilde{c} + (1-\tilde{\Phi})\right]\tilde{u}_\mu = \mu^\alpha\tilde{\Phi}\tilde{f} + (1-\tilde{\Phi})A,$$

$$\tilde{u}_\mu(-1) = \alpha_1, \quad \tilde{u}_\mu(\theta+1) = \alpha_2,$$

— a *singularly perturbed boundary value problem* for $\alpha > 2$.

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Thus, for $\xi \in [0, \theta]$ the function $\tilde{u}_\mu$ matches the solution of the problem

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Thus,

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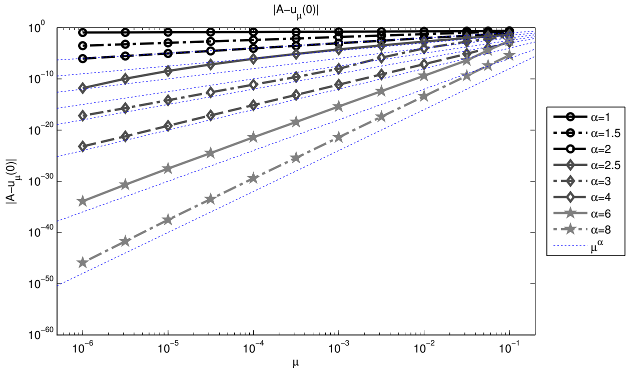

Fulfilment of the condition $u_\mu(0) \approx A$ for various values of α

Analysis – Step 3

Proposition

For $\alpha > 2$ and $\mu < \mu_0$, where μ_0 is sufficiently small, we have

$$|u_\mu(x) - A| \leq C\mu \text{ and } |u'_\mu(x)| \leq C \text{ for } x \in \left[\theta\mu, \frac{\alpha-2}{2}\mu|\ln\mu|\right].$$

Remark to Proposition The scaled differential equation

$$-\mu^{\alpha-2}\frac{\partial}{\partial\xi}\left(\tilde{\Phi}\frac{\partial}{\partial\xi}\tilde{u}_\mu\right) + \left[\mu^\alpha\tilde{\Phi}\tilde{c} + (1-\tilde{\Phi})\right]\tilde{u}_\mu = \mu^\alpha\tilde{\Phi}\tilde{f} + (1-\tilde{\Phi})A$$

changes its behaviour at $t = \frac{\alpha-2}{2}|\ln\mu|$ because

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Remark to Proposition, cont. In the interval $[\theta, \beta t]$ with $0 < \beta < 1$, it can be analysed as boundary-value problem and we obtain

$$u_\mu = A + \mathcal{O}\left(\mu^{\alpha(1-\beta)+2\beta}\right) + \Psi,$$

where Ψ is a layer term of the structure

$$\Psi(\xi) = \mathcal{O}\left(\exp\left(-\frac{t-\xi}{\mu^{\frac{(\alpha-2)(1-\beta)}{2}}}\right)\right).$$

Thus, for $\xi \in [\theta, \tilde{\beta} t]$ with $0 < \tilde{\beta} < \beta < 1$, we observe $u_\mu - A = \mathcal{O}\left(\mu^2\right)$ if μ is sufficiently small. But the *layer term Ψ dominates* for larger ξ and numerically we observe near $\xi = t$ only $u_\mu - A = \mathcal{O}(\mu)$.

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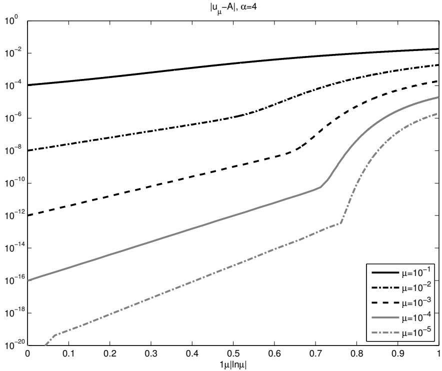

Behaviour of $|u_\mu - A|$ in $[0, \mu|\ln\mu|]$ for $\alpha = 4$

Analysis – Step 4

Lemma

Assume the previous proposition holds true. For $\alpha > 2$ and $\mu < \mu_0$, where μ_0 is sufficiently small, we have

$$|u_\mu(x) - A| \leq C\mu^{1-\varepsilon} \quad \textit{in} \quad \left[\frac{\alpha-2}{2}\mu|\ln\mu|, \frac{\alpha-1}{2}\mu|\ln\mu|\right],$$

where $\varepsilon > 0$ is arbitrarily small.

Proof. Idea: Consider the differential problem as *initial value problem* for $\hat{w} = \frac{\hat{u}_\mu - A}{\mu^2|\ln\mu|^2}$ and use initial values gained by the proposition. Then, *bounds on the growth* of $\hat{w}$ give the result.

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Analysis – Step 2-4 combined

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Numerically we observe the slightly better result

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Corollary

From the previous steps we obtain for $x \in [0, \frac{\alpha-1}{2}\mu|\ln\mu|]$

$$|u(x) - u_\mu(x)| \leq |u(x) - u(0)| + |u_\mu(x) - A| \leq C\mu^{1-\varepsilon}$$

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If $\alpha > 2$ and $\mu < \mu_0$ where μ_0 is sufficiently small, then follows that

$$|(u - u_\mu)(x)| \le C\mu^{1-\varepsilon} \quad \text{in } [x_k, 1],$$

where $x_k = (\alpha - 1)\mu|\ln \mu|/2$.

Proof. The difference $w := u - u_\mu$ suffices in the interval $(x_k, 1]$ the boundary value problem (recall $Lu = -u'' + cu = f$)

$$Lw = \frac{1-\Phi}{\mu^\alpha \Phi}(u_\mu - A) + \frac{2}{\mu}(1-\Phi)u'_\mu =: h(x),$$

$$w(x_k) = \mathcal{O}\left(\mu^{1-\varepsilon}\right), \quad w(1) = 0.$$

Using a *Green's function representation* of w, bounds on $G(x,t)$ and $G_t(x,t)$, h being small due to $1 - \Phi(t) \le C\exp(-2t/\mu)$ we are done.

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$$w(x_k) = \mathcal{O}\left(\mu^{1-\varepsilon}\right), \quad w(1) = 0.$$

Using a *Green's function representation* of w, bounds on $G(x,t)$ and $G_t(x,t)$, h being small due to $1 - \Phi(t) \leq C\exp(-2t/\mu)$ we are done.

Analysis – Step 5

Lemma

If $\alpha > 2$ and $\mu < \mu_0$ where μ_0 is sufficiently small, then follows that

$$|(u - u_\mu)(x)| \le C\mu^{1-\varepsilon} \quad \text{in } [x_k, 1]\,,$$

where $x_k = (\alpha - 1)\mu|\ln \mu|/2$.

Proof. The difference $w := u - u_\mu$ suffices in the interval $(x_k, 1]$ the boundary value problem (recall $Lu = -u'' + cu = f$)

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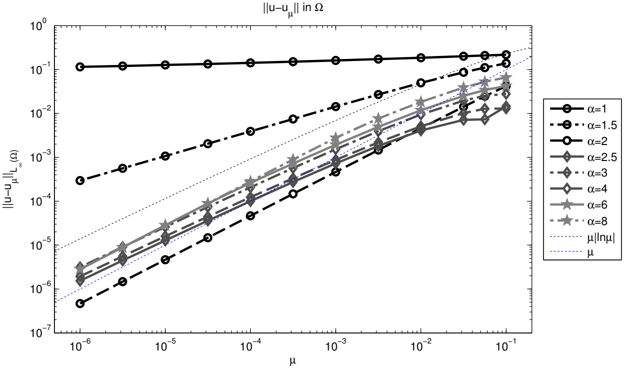
Analysis



Convergence of u_μ to u for various values of α.

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Open questions:

- How to prove the proposition?
- Can the convergence result $|u - u_\mu| \leq C\mu^{1-\varepsilon}$ be improved to $|u - u_\mu| \leq C\mu|\ln\mu|$?
- Is there a simpler proof? $\Rightarrow$ Better understanding of the behaviour of the method is needed.
- Extension to more than one dimension and more complicated domains.

Thank you for your attention.

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